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Note

A Rational Approximation for the Exponential Appearing in the Theory of Thermally Stimulated Processes

In the first-order theory of thermally stimulated processes, (TSP), such as thermoluminescence (TL), thermally stimulated depolarization (TSD), etc., one meets the equation for a single peak,

$$I = n_0 s \exp\left\{-\frac{E}{kT} - \int_0^T \frac{s}{\beta} \exp\left(-\frac{E}{kT'}\right) dT'\right\}. \tag{1}$$

In the case of TL, n_0 is the number of charge carriers (electrons or holes) initially trapped in traps characterized by an energy depth E and a frequency factor s, the rate at which the temperature is increased is $\beta = dT/dt$ and $I = -dn/dt$ is the rate at which electrons are liberated from the traps. k is Boltzmann's constant. The equation is known in TL as the Randall–Wilkins equation.

In TSD, n_0 is replaced by Q_0, the total charge initially present at each of the sample's faces when it is polarized, $1/s$ is represented by the preexponential factor (time constant) τ_0 and I is the depolarization current being released during heating. This symbolism may also be used in TL if it is assumed that the photomultiplier current output which is proportional to the emitted light intensity is in turn proportional to $-dn/dt$, in which case Q_0 will be the total electric charge to be finally collected (i.e., the area under the peak when the current I is plotted as a function of time).

Equation (1) is simplified if s is temperature independent. If in addition β is constant (linear heating), the quantity s/β may be taken outside the integral. By differentiation it is found that the peak maximum occurs at a temperature T_M satisfying the equation

$$\frac{\beta E}{kT_M^2} = s \exp\left(-\frac{E}{kT_M}\right). \tag{2}$$

Using the variable $\varepsilon = E/kT$ and its value $\varepsilon_M = E/kT_M$ at peak maximum, (1) and (2) give for the height of the peak [1]

$$I_M = \frac{\beta n_0}{T_M} \varepsilon_M \exp\{-\varepsilon_M e^{\varepsilon_M} E_2(\varepsilon_M)\}, \tag{3}$$

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where

$$E_2(\varepsilon) = \int_1^\infty \frac{e^{-\varepsilon t}}{t^2}\, dt.$$

Series expansions exist for $E_2(\varepsilon)$ [2] and considerable work has been done in expressing the function by rational expressions [2–12] for use in numerical work.

Methods of data analysis exist [13, 14], which make use of the peak height $I_M = I(\varepsilon_M)$ for the determination of the parameters E and s. To facilitate the use of these methods, it is required that a rational approximation is found for the exponential in (3). One such approximation [14], found by using the first term in the asymptotic expansion

$$E_2(x) \sim \frac{e^{-x}}{x}\left\{1 - \frac{2!}{x} + \frac{3!}{x^2} - \frac{4!}{x^3} + \cdots\right\} \tag{4}$$

is not accurate enough since in thermally stimulated processes ε_M can be as low as 10 or 15, in which cases the error in the exponent of (3) can be as high as 0.15, leading to the overestimation of ε_M and E by a factor of up to 1.16. This in turn leads to s values which are up to 7 times the actual values when (2) is used.

It will be shown below that quite an accurate expression can be obtained for the exponential in (3) by using the series expansion [2]

$$E_2(x) = \frac{e^{-x}}{x+2}\left\{1 + \frac{2}{(x+2)^2} - \frac{4(x-1)}{(x+2)^4} + \cdots\right\}. \tag{5}$$

The function defined as

$$L(x) = 1 - xe^x E_2(x) \tag{6}$$

decreases monotonically from the value of 0.1563 for $x = 10$ to zero for $x \to \infty$. Using (5) for $E_2(x)$ in (6) it is found that

$$\exp\{L(x)\} = \frac{x+4}{x+2} + \frac{16}{3(x+2)^3} + \cdots \tag{7}$$

or, since the values of interest of ε_M in thermally stimulated processes are higher than 10 or 15, to a good approximation,

$$\exp\{L(x)\} = \exp\{1 - xe^x E_2(x)\} \approx \frac{x+4}{x+2}. \tag{8}$$

With this approximation, (3) becomes

$$I_M \approx \frac{\beta n_0}{eT_M}\, \varepsilon_M \frac{\varepsilon_M + 4}{\varepsilon_M + 2} \tag{9}$$

TABLE I

Comparison of Approximate and Exact Values of the Function $\exp\{L(x)\}$

x	$L(x)$	$\left(\frac{x+4}{x+2}\right)\Big/\exp\{L(x)\}$	$\left(\frac{x+3.740}{x+1.752}\right)\Big/\exp\{L(x)\}$
10	0.156 334	0.997 819	0.999 954
12	0.134 963	0.998 569	1.000 058
15	0.112 063	0.999 163	1.000 080
20	0.087 418	0.999 594	1.000 038
25	0.071 686	0.999 773	0.999 995
30	0.060 764	0.999 860	0.999 964
40	0.046 584	0.999 936	0.999 932
50	0.037 775	0.999 965	0.999 920
100	0.019 425	0.999 993	0.999 924

which is a rational approximation accurate enough for the determination of ε_M in terms of I_M and the other parameters of (9) [15].

The errors introduced in $\exp\{L(x)\}$ by the approximation (8) are shown in Table I. It is seen that these errors are negligible for all practical purposes for $\varepsilon_M \geqslant 10$ and even more so for $\varepsilon_M \geqslant 15$ which is true in most cases met in the phenomena of TL and TSD, and most TSP, in general. Better accuracy is not needed in experimental work in thermally stimulated processes, but an expression more accurate than (8) may be obtained, namely,

$$\exp\{L(x)\} = \exp\{1 - xe^x E_2(x)\} \approx \frac{x+3.740}{x+1.752}. \tag{10}$$

The maximum absolute error due to this expression for $x \geqslant 10$ is 80 ppm. The ratio of the approximate values of $\exp\{L(x)\}$ from (10) to the actual ones are also given in Table I.

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